# Using lattice methods in non-canonical quantum statistics

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We define a natural coarse-graining procedure which can be applied to any closed equilibrium quantum system described by a density matrix ensemble and we show how the coarse-graining leads to the Gaussian and canonical ensembles. After this motivation, we present two ways of evaluating the Gaussian expectation values with lattice simulations. The first one is computationally demanding but general, whereas the second employs only canonical expectation values but it is applicable only for systems which are almost thermodynamical.

## 1. Introduction

The usefulness of the canonical ensemble in statistical mechanics is remarkable. The standard explanation of this success relies in taking the "thermodynamical limit" which corresponds to increasing the volume of the system to infinity while keeping all the relevant intensive quantities, i.e. densities, fixed and finite. From this point of view, the canonical ensemble should not have much utility for small systems consisting of only a few particles. This, however, does not seem to be the case, and in the following we propose a new approach which explains why and how the canonical ensemble can help also in the analysis of small equilibrium systems. We also explain how lattice simulations in general can be employed in this analysis.

## 2. Ensembles from coarse-graining of the energy fluctuation spectrum

The standard approach to quantum statistics [1] uses a density matrix $\widehat{\rho}$, which is a non-negative, hermitian, trace class operator normalized to one and which gives the expectation value of an observable $\widehat{A}$ by the formula $\langle\widehat{A}\rangle = \mathrm{Tr}\,(\widehat{A}\widehat{\rho})$. In some complete eigenbasis $|\psi_i\rangle$, the density matrix can thus be expanded as $\widehat{\rho} = \sum_i p_i|\psi_i\rangle\langle\psi_i|$, where the eigenvalues $p_i$ satisfy $p_i \geq 0$ and the normalization condition $\sum_i p_i = 1$.

Suppose now that the system has a discrete energy spectrum, which in quantum mechanics is achieved for every potential that grows sufficiently fast at infinity. An equilibrium, i.e. time-independent, ensemble is then given by a density matrix which has time-independent eigenvalues and which satisfies $[\widehat{H}, \widehat{\rho}] = 0$. In this case, the eigenvectors $\psi_i$ can be chosen so that they are also energy eigenvectors with an eigenvalue $E_i$.

After these preliminaries, it is not hard to see that for *any* equilibrium ensemble which is given by a density matrix and which has energy as the only relevant conserved quantity, we can find a smooth mapping $F$ so that $\widehat{\rho} = F(\widehat{H})$, i.e. that $\widehat{\rho} = \sum_i F(E_i)|\psi_i\rangle\langle\psi_i|$. We will call such a smooth mapping the *fluctuation spectrum* of the ensemble and we will use the term *precanonical ensemble* for those equilibrium ensembles which satisfy:

1. The canonical partition function converges, $\mathrm{Tr}\,\mathrm{e}^{-\beta\widehat{H}} < \infty$, for all $\beta > 0$.

2. The energy fluctuations decay at least exponentially at high energies: $\mathrm{e}^{\beta E}F(E)$ is a rapidly decreasing function [2] for all $\beta < \beta_+$, where $\beta_+ > 0$ is a parameter.

The following representation is then valid for any precanonical ensemble and for all $0 < \beta < \beta_+$ as long as $\widehat{A}$ is a positive observable which satisfies $\mathrm{Tr}\,[\widehat{A}\mathrm{e}^{-\beta\widehat{H}}] < \infty$ in the same range of $\beta$:

$$\mathrm{Tr}\big[\widehat{A}F(\widehat{H})\big] = \int_{\beta-\mathrm{i}\infty}^{\beta+\mathrm{i}\infty}\frac{\mathrm{d}w}{2\pi\mathrm{i}}\bar{F}(w)\mathrm{Tr}\big[\widehat{A}\mathrm{e}^{-w\widehat{H}}\big], \quad (1)$$

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where $\bar{F}$ is the Laplace transform of $F$ and the integrand in the above equation is an analytic function in the half-plane $0 < \mathrm{Re}\, w < \beta_+$. This result follows from Fourier-transform formulae for rapidly decreasing functions; the precise mathematical details can be found from [3].

The value of the integral representation (1) can be computed by saddle point methods and, for instance when $\widehat{A} = \widehat{1}$, there is a unique positive saddle point $\beta$ which dominates the value of the integral. For $\widehat{A} = \widehat{1}$ it can be solved for small $\beta$ from the saddle point equation

$$\langle \widehat{H} \rangle_\beta^{\mathrm{can}} = E + \beta\varepsilon^2 + \mathcal{O}(\beta^2), \tag{2}$$

where, assuming the normalization $\int F = 1$,

$$E = \int \mathrm{d}x F(x) x, \quad \varepsilon^2 = \int \mathrm{d}x F(x)(x-E)^2. \tag{3}$$

Since the precise form of the fluctuation spectrum is difficult to measure, we need some way of parameterizing its large scale properties. As usual, these can be extracted from the original fluctuation spectrum by a coarse-graining transformation—here we used a convolution with a Gaussian distribution,

$$F(x) \mapsto F_\Lambda(x) \equiv \int_{-\infty}^{\infty} \mathrm{d}y F(y) \frac{1}{\sqrt{2\pi\Lambda^2}} \mathrm{e}^{-\frac{1}{2\Lambda^2}(x-y)^2}.$$

Under this transformation, the Laplace-transform in (1) will change to $\bar{F}_\Lambda(w) = \mathrm{e}^{\frac{1}{2}\Lambda^2 w^2} \bar{F}(w)$.

When $\Lambda$ approaches infinity it is clear that the positive saddle point value $\beta$ must go to zero. Since $\bar{F}_\Lambda$ is analytic near the origin, we can in this limit use the approximation $Ew + \frac{1}{2}\varepsilon^2 w^2$ for $\ln \bar{F}_\Lambda(w)$—the parameters are obtained from (3) by replacing $F$ with $F_\Lambda$. Taking the inverse Laplace-transform then shows that this corresponds to using the Gaussian ansatz $F_\Lambda(x) = G_\varepsilon(E - x)$ for the fluctuation spectrum. This should not come as a surprise; the argumentation is the same as used with the central limit theorem of probability theory.

For large $\Lambda$ the positive saddle point typically becomes dominant. On the other hand, the trace left in the positive saddle point approximation is simply the canonical trace, $\mathrm{Tr}\,(\widehat{A}\mathrm{e}^{-\beta\widehat{H}})$, and often the canonical expectation value becomes a good approximation of the coarse-grained one. The precise condition for the use of the canonical ensemble can be given in terms of the canonical variance $\sigma^2 = \langle (\widehat{H} - \langle \widehat{H} \rangle)^2 \rangle_\beta^{\mathrm{can}}$ and the normalized canonical energy operator $\widehat{h} = (\widehat{H} - \langle \widehat{H} \rangle)/\sigma$. The condition for using the canonical approximation for the partition function and the one for using the canonical expectation value for a positive observable $\widehat{A}$ are, respectively,

$$a \equiv \frac{\sigma^2}{2\varepsilon^2} \ll 1 \quad \text{and} \quad a\langle \widehat{A}\widehat{h}^2 \rangle / \langle \widehat{A} \rangle \ll 1.$$

Similarly, the Gaussian ensemble can be used if the left hand sides in the previous equations are not too large. A more complete explanation of these results can be found in [3].

The canonical approximation of the Gaussian expectation values has already been analysed in [4] and we quote here only the results: The simple bounds, already referred to in the above, for the approximation of positive observables are

$$-a\frac{\langle \widehat{A}\widehat{h}^2 \rangle}{\langle \widehat{A} \rangle} \leq \ln \frac{\langle \widehat{A} \rangle_{E,\varepsilon}^{\mathrm{gauss}}}{\langle \widehat{A} \rangle_\beta^{\mathrm{can}}} \leq a$$

and this approximation can be improved for $a \approx 1$ by using the asymptotic series

$$\langle \widehat{A} \rangle_{E,\varepsilon}^{\mathrm{gauss}} = \langle \widehat{A} \rangle_\beta^{\mathrm{can}} + \langle (1 - \widehat{h}^2)\widehat{A} \rangle a + \mathcal{O}(a^2). \tag{4}$$

## 3. Gaussian ensemble on a lattice

There are two different ways of using lattice simulations in the evaluation of Gaussian expectation values. In the direct approach, the lattice approximation is applied to the complex temperature trace in (1) which, after an exchange of the order of the integration and the continuum limit, leads to an integral kernel for the lattice simulations. Unfortunately the kernel is not a positive function and the results are in most cases obtained as a delicate cancellation of oscillations of the kernel. This, however, is likely to be an unavoidable feature of any space-lattice simulation of microcanonical expectation values as the energy wavefunctions themselves are typically highly oscillatory.

This approach is most useful when canonical simulations at a complex temperature are possible. Then the trace in the the integrand in (1)

can be evaluated in a number of points and the integral computed by a discrete Fourier-transform. This would yield results for a range of values of the parameters $E$ and $\varepsilon$ and, therefore, it would enable an inspection of a whole energy range at the same time. The main difficulty in this approach is, of course, in the complex temperature lattice simulation with its oscillatory kernel function.

If an expectation value at only one value of the parameters $E$ and $\varepsilon$ is needed, then a second alternative is also possible: perform first the Fourier-transformation of the canonical lattice kernel and do the lattice simulations with the resulting kernel function. In this case, the evaluation of the kernel function becomes an obstacle slowing down the simulation.

The second approach to the Gaussian evaluation problem is to use the asymptotic series given in (4) which requires the computation of *canonical* expectation values only. The problem in this case is to find the correct lattice operators which would correspond to the different powers of $\widehat{h}$ in the continuum limit. We will now show how these can be found in a simple quantum mechanical case and comment on some general features which should be relevant also for field theory lattice simulations—a more complete analysis of this kind of lattice system can be found from [5].

Consider, for simplicity, a non-relativistic particle in a potential $V(x)$. The Hamiltonian of this system is $\widehat{H} = \frac{1}{2m}\widehat{p}^2 + V(\widehat{x})$ and if the potential is bounded from below and increases sufficiently fast at infinity, the complex temperature trace has a rigorous lattice approximation given by

$$\mathrm{Tr}\,\mathrm{e}^{-w\widehat{H}} = \lim_{L\to\infty}\int \mathrm{d}^L x [L/(2\pi w)]^{L/2} \mathrm{e}^{-\frac{1}{w}P_L - wV_L},$$

$$P_L = \frac{L}{2m}\sum_{k=1}^{L}|x_{k-1}-x_k|^2\,,\; V_L = \frac{1}{L}\sum_{k=1}^{L}V(x_k).$$

A straightforward differentiation of this result then gives the operators which will measure in the continuum limit the expectation values of different powers of the Hamiltonian. We have given the first few of them in Table 1. Two features of these results are worth pointing out: first, the kinetic energy is given by the operator $\frac{1}{2}L - \frac{1}{\beta}P_L$, which shows that $P_L$ diverges as the lattice size in the continuum limit and thus needs to be "renormalized". This reflects the well-known result that the continuum path-integral is concentrated on paths which are continuous, but non-differentiable. Secondly, each power of the Hamiltonian needs a separate renormalization term in the sense that using the powers of the operator giving the expectation value, $c_1$, is not enough. This is exactly analogous to the situation of composite operators in field theory.

Table 1
Lattice energy operators in terms of $M = L/2$, $P_\beta = \frac{1}{\beta}P_L$ and $V_\beta = \beta V_L$.

| | |
|---|---|
| "$\beta H$" $= c_1$ | $c_1 = M - P_\beta + V_\beta$ |
| "$\beta^2 H^2$" $= c_1^2 + c_2$ | $c_2 = M - 2P_\beta$ |
| "$\beta^3 H^3$" $= c_1^3 + 3c_1c_2 + c_3$ | $c_3 = 2(M - 3P_\beta)$ |

## 4. Conclusions

We have introduced the Gaussian ensemble as a means of refining the accuracy of the canonical ensemble and we have shown by a coarse-graining procedure why this would have applications also for non-thermal equilibrium systems. The canonical, complex temperature, lattice simulations offer one way of inspecting the behavior of the Gaussian expectation values. A second way, applicable for systems near the thermodynamical limit, uses correction terms which can be computed with the well-established methods of canonical lattice simulations.

## REFERENCES


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